

DCPT: A Dual-Continua Random Walk Particle Tracker for Transport

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Research Objectives

Accurate and efficient simulation of chemical transport processes in the unsaturated zone of Yucca Mountain is important to evaluate the performance of the potential repository. The scale of the unsaturated zone model domain for Yucca Mountain (50 km² area with a 600 meter depth to the water table) requires a large gridblock approach to efficiently analyze complex flow & transport processes. The conventional schemes based on finite element or finite difference methods perform well for dispersion-dominated transport, but are subject to considerable numerical dilution/dispersion for advection-dominated transport, especially when a large gridblock size is used. Numerical dispersion is an artificial, grid-dependent chemical spreading, especially for otherwise steep concentration fronts.

One effective scheme to deal with numerical dispersion is the random walk particle method (RWPM). While significant progress has been made in developing RWPM algorithms and codes for single continuum systems, a random walk particle tracker, which can handle chemical transport in dual-continua (fractured porous media) associated with irregular grid systems, is still absent (to our knowledge) in the public domain. This is largely due to the lacking of rigorous schemes to deal with particle transfer between the continua, and efficient schemes to track particles in irregular grid systems. The main objectives of this study are (1) to develop approaches to extend RWPM from a single continuum to a dual-continua system; (2) to develop an efficient algorithm for tracking particles in 3D irregular grids; and (3) to integrate these approaches into an efficient and user-friendly software, DCPT, for simulating chemical transport in fractured porous media.

Approach

In RWPM, chemical transport is represented by movement of a large number of particles. In addition to advection determined by the corresponding velocity field, dispersion/diffusion is simulated by random walks of particles. In DCPT, RWPM is directly adopted to simulate particle movement in each continuum. Unlike a single continuum, however, a dual-continua system is associated with two very different velocity fields at a given "physical point". The mass transfer between the fracture and matrix

continua is one of the critical processes that control the movement of chemicals. The mass transfer process between the fracture and the matrix is simulated by the particle transfer probabilities (PTP) which determine if a particle will leave the current continuum at next time level. Determination of PTP is one of the key & unique elements in DCPT.

The challenge is to convert the net mass flow between the fracture and the matrix (in the Eulerian point of view) into the particle transfer probabilities (the Lagrangian point of view). An analytical solution of the mass conservation equation of the particles (in the Lagrangian point of view) is found, based on which a new scheme to calculate the PTP is developed and incorporated into DCPT (Pan et al., 1999).

In most of the currently available RWPM codes, regular grids are generally used. For many subsurface contaminant problems, such as those in the unsaturated zone of Yucca Mountain, the related subsurface media can be highly heterogeneous. To capture these heterogeneities, irregular grid systems are required. An efficient scheme to track particle locations in irregular grids was developed for DCPT (Pan et al., 1999). The main idea of this scheme is to establish a secondary structure of the original 3D irregular grid so that only a very small portion of the whole grid has to be searched each time. This can avoid decaying of the computational efficiency due to increases in the number of grid blocks.

DCPT can be used to simulate reactive transport with linear sorption. For a single continuum system, the retardation factor method has been widely used in RWPM. However, this approach can not be directly used for a dual-continua system, because of the coupling of transport processes in the two continua with different retardation factors. In the light of the imaginary porosity method proposed by Liu and Bodvarsson (1999), a physically based conditional probability approach (Pan et al., 1999) was incorporated into

DCPT to describe the effects of the linear sorption process on either the transfer probability between two continua or the advection/dispersion processes in each continuum.

DCPT was developed using FORTRAN 90 and following the principle of the objective-oriented programming technologies.

Results

Figure 1 shows comparisons between simulation results of DCPT and several typical analytical solutions in 1D and 2D domains. The comparisons were designed to verify DCPT's capability to calculate particle transfer between the two continua and consider the sorption (Figure 1a), to incorporate dispersion and diffusion in multi-dimensional domains (Figure 1b), and to track particle movement in an irregular grid (Figure 1c). Particularly, figure 1c depicts a trail of a particle in a concentric velocity field (radial velocity is zero everywhere) simulated by DCPT, which is a circle theoretically. The satisfactory matches indicate that the methodologies and algorithms developed are valid and successful.

Figure 2 shows comparison between simulation results obtained from DCPT (2000 particles) and T2R3D (Wu et al., this report) for two 1D problems under unsaturated conditions. The corresponding 1D column is extracted from the 3D grid of the site-scale unsaturated zone (UZ) model for Yucca Mountain. The comparison is fairly good, and DCPT gives a steeper concentration front, resulting from its ability to deal with numerical dispersion.

All the simulations of DCPT mentioned above were performed on a Pentium II 300 MHz PC and took a few seconds up to about 10 minutes of CPU time, depending the particle numbers used.

Significance of Findings

Based on the newly developed methodologies to extend RWPM from a single continuum system to a dual continua system, a new software program, DCPT, has been developed. Comparisons between DCPT simulation results with analytical solutions and results obtained from T2R3D show that DCPT could be used to simulate chemical transport processes associated with linear sorption in fractured continua without numerical dispersion.

Related Publications

Liu, H.H., and G.S. Bodvarsson, A scheme to determine particle transfer in random walk algorithms for dual continua, *Water Resour. Res.*, in review; LBNL-43358, Lawrence Berkeley National Laboratory, Calif., 1999.

Pan, L., H.H. Liu, M. Cushey, and G.S. Bodvarsson, DCPT: A new random walk particle tracker for dual-continua,

LBNL-42958, Lawrence Berkeley National Laboratory, Calif., 1999.

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